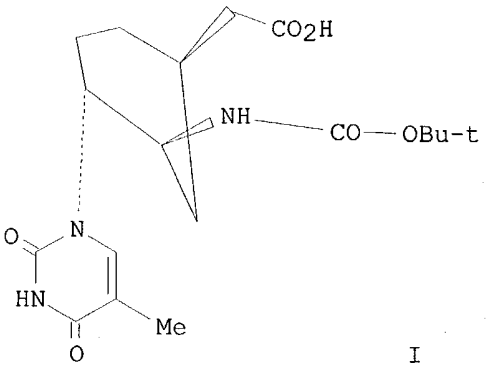
=> d ibib abs hitstr l12 1-15

L12 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:153401 HCAPLUS
DOCUMENT NUMBER: 138:188074
TITLE: Synthesis of cyclohexyl- or hetero-cyclohexyl-nucleosides and their oligomers or conjugates
INVENTOR(S): Reuschling, Dieter; Muller-Ibeler, Jochen; Wagner, Thomas; Krumm, Thomas; Wermuth, Jochen; Pignot, Marc
PATENT ASSIGNEE(S): Nanogen Recognomics GmbH, Germany
SOURCE: Ger. Offen., 32 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10139730	A1	20030227	DE 2001-10139730	20010813
WO 2003016561	A2	20030227	WO 2002-EP9044	20020813
WO 2003016561	A3	20031204		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: DE 2001-10139730 A 20010813
OTHER SOURCE(S): MARPAT 138:188074
GI



I

AB Cyclohexane-based peptide nucleic acid monomer analogs (CNA-monomers, e.g., I) or their enantiomers were prepared Oligomers of CNA monomers were prepared using solid-phase synthesis techniques. A fluorescently labeled CNA pentamer was hybridized with a biotin-labeled pseudo-nucleic acid

octamer with a phosphate-bridged backbone composed of 2→4-ribo-pyranose for thermal decomposition study on base-pairing of the two dissimilar nucleic acid analogs. Thus, thymine was condensed with (1R,5R,8R)-8-iodo-2-azabicyclo[3.3.1]nonan-3-one, the intermediate's secondary amine nitrogens were BOC-protected, the lactam bond cleaved, and the thymine-base ring nitrogen BOC group removed to give I. Addnl., preparation and use of H2O3PO(CH2)3CO2H for use as the N-terminal protecting group in CNA-oligomers was given.

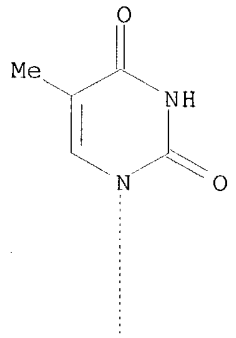
IT **497944-45-3P 497944-46-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of cyclohexyl-nucleoside derivs. and their oligomers or conjugates via base coupling to iodoazabicyclononanone followed by ring-opening)

RN 497944-45-3 HCAPLUS

CN Glycine, N2-[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-(acetylamino)-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]-N6-(iodoacetyl)-L-lysyl-L-cysteinyl-L-seryl-L-lysyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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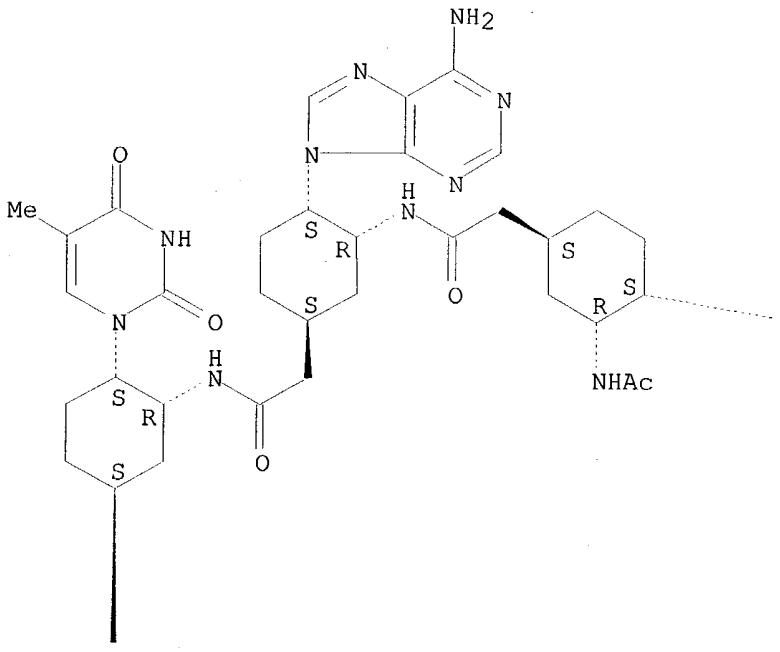

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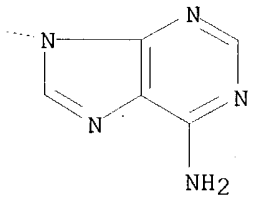

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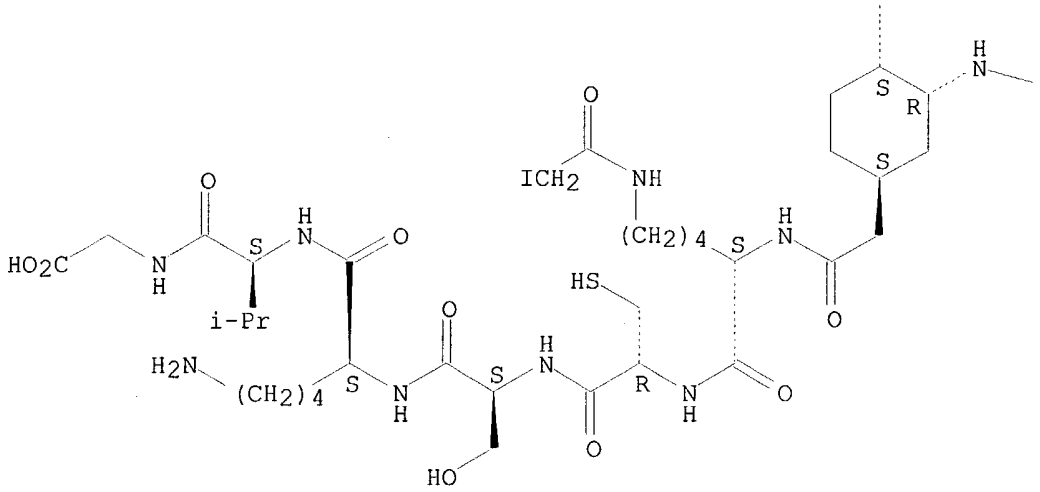

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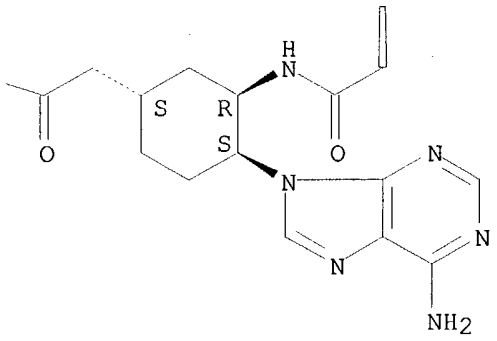
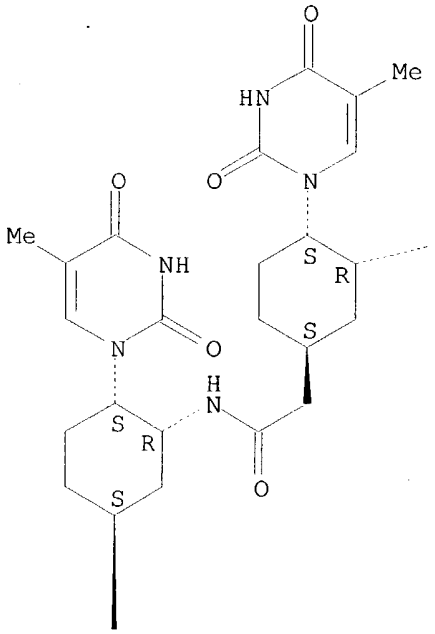


RN 497944-46-4 HCAPLUS
CN L-Lysinamide, L-cysteinyl-L-alanyl-L-alanyl-L-alanylglycyl-N-[(1R,2S,5S)-5-[2-[[(1R,2S,5S)-5-[2-[[(1R,2S,5S)-5-[2-[[(1R,2S,5S)-5-[2-[[(1R,2S,5S)-5-(carboxymethyl)-2-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]amino]-2-oxoethyl]-2-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]amino]-2-oxoethyl]-2-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]amino]-2-oxoethyl]-2-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]amino]-2-oxoethyl]-2-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]-N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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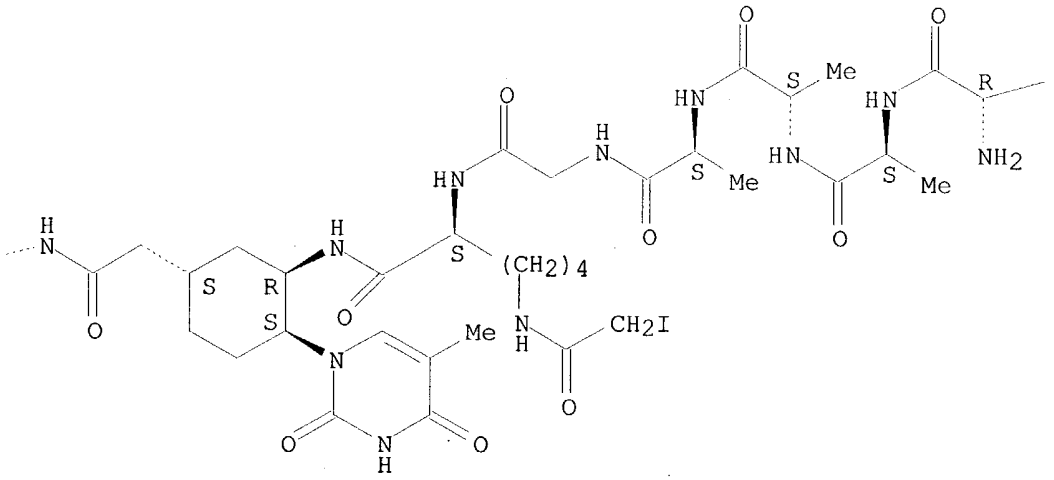

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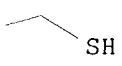

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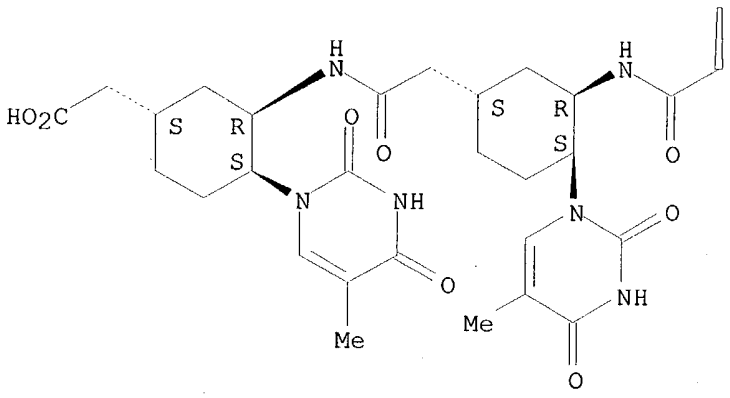


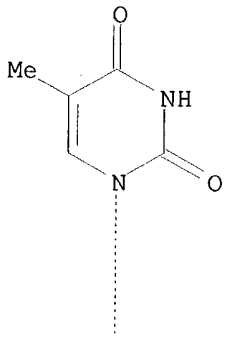
IT **497944-39-5P 497944-40-8DP**, resin-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclohexyl-nucleoside derivs. and their oligomers or conjugates via base coupling to iodoazabicyclononanone followed by ring-opening)

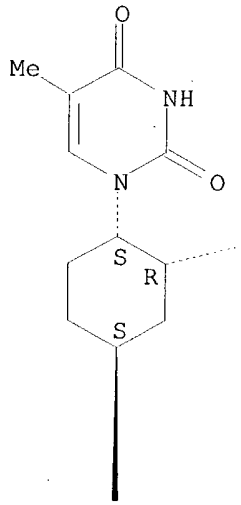
RN 497944-39-5 HCAPLUS

CN L-Lysine, N2-[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-(acetylamino)-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-[3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl]cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-[3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl]cyclohexyl]acetyl]-N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





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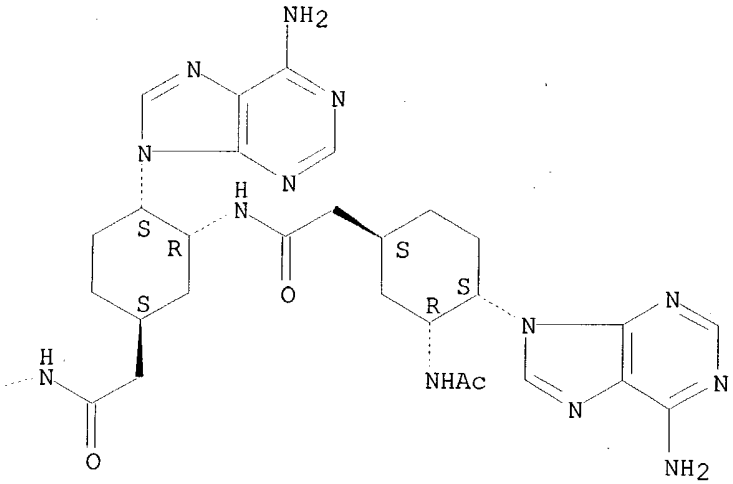

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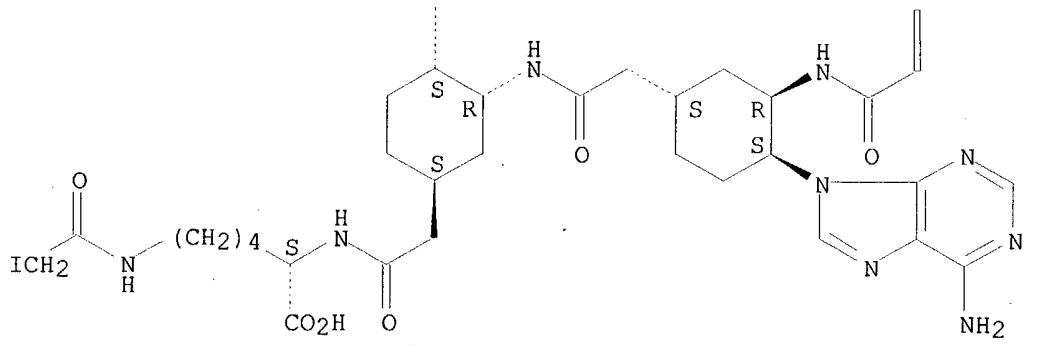
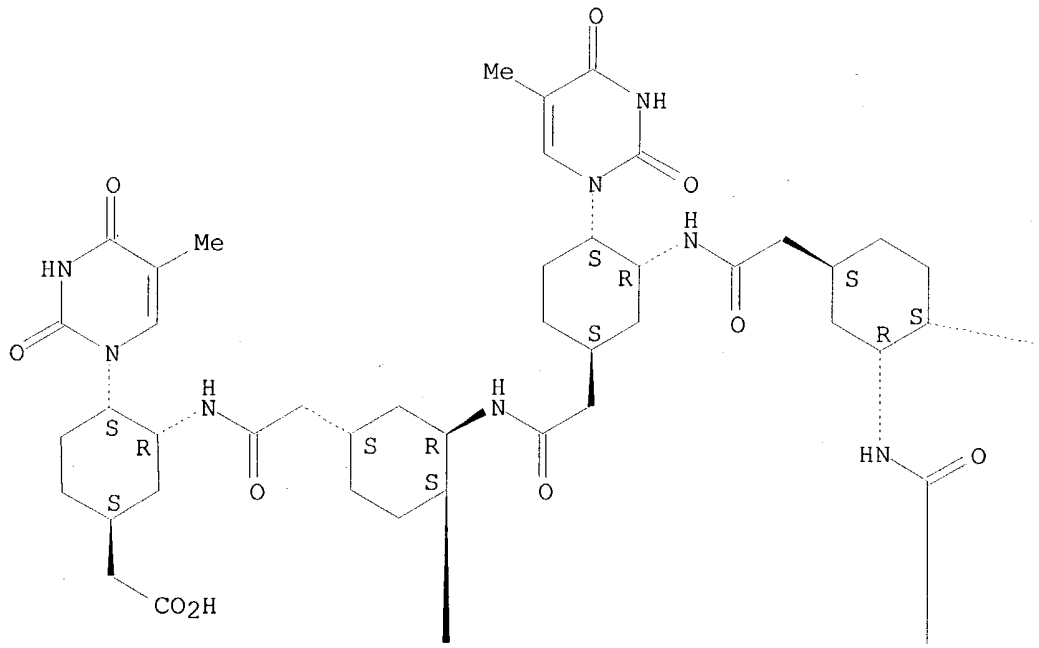


RN 497944-40-8 HCAPLUS

CN Cyclohexaneacetic acid, 3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[[(1S,3R,4S)-3-[[(2S)-2-amino-6-[(iodoacetyl)amino]-1-oxohexyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-, (1S,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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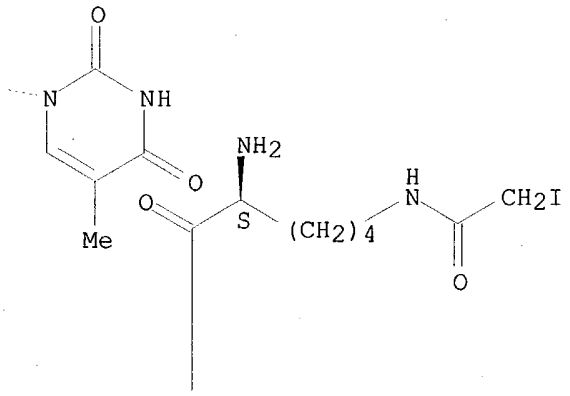

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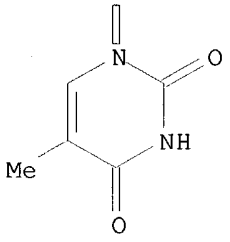

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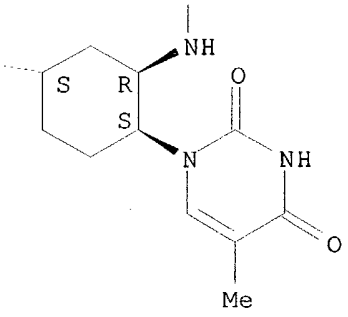


L12 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:241074 HCAPLUS
DOCUMENT NUMBER: 136:272403
TITLE: Automated system for two-dimensional electrophoresis
INVENTOR(S): Goodman, Jack; Anderson, N. Leigh
PATENT ASSIGNEE(S): Large Scale Proteomics Corporation, USA
SOURCE: PCT Int. Appl., 82 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002025259	A2	20020328	WO 2001-US26085	20010821
WO 2002025259	A3	20021010		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 6554991	B1	20030429	US 2000-667567	20000921
AU 2001086582	A5	20020402	AU 2001-86582	20010821
GB 2384206	A1	20030723	GB 2003-8977	20010821

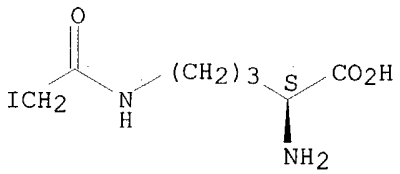
PRIORITY APPLN. INFO.:
US 2000-667567 A 20000921
US 1997-881761 A3 19970624
US 1999-339164 A2 19990624
WO 2001-US26085 W 20010821

AB The present invention provides an integrated, fully automated, high-throughput system for two-dimensional electrophoresis comprised of gel-making machines, gel processing machines, gel compns. and geometries, gel handling systems, sample preparation systems, software and methods. The system is capable of continuous operation at high-throughput to allow construction of large quant. data sets.

IT **35748-65-3**, L-Ornithine, N5-(iodoacetyl)-
RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(alkylating agent; automated system for two-dimensional gel electrophoresis anal. of sulfhydryl group-containing proteins)

RN 35748-65-3 HCAPLUS
CN L-Ornithine, N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:819185 HCAPLUS
DOCUMENT NUMBER: 132:61295

TITLE: Novel compounds
INVENTOR(S): Leach, Colin Andrew; Moore, Keith James Millan; Stanway, Steven James
PATENT ASSIGNEE(S): Smithkline Beecham Plc, UK
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9966780	A2	19991229	WO 1999-EP4277	19990618
WO 9966780	A3	20000203		
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2335610	AA	19991229	CA 1999-2335610	19990618
EP 1090007	A2	20010411	EP 1999-931117	19990618
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002518413	T2	20020625	JP 2000-555481	19990618
US 6441167	B1	20020827	US 2001-720172	20010216

PRIORITY APPLN. INFO.: GB 1998-13776 A 19980625
WO 1999-EP4277 W 19990618

AB This invention relates to novel compds. that can complex with lanthanide cations, processes for their preparation and the use of the resulting lanthanide chelates as biomol. probes.

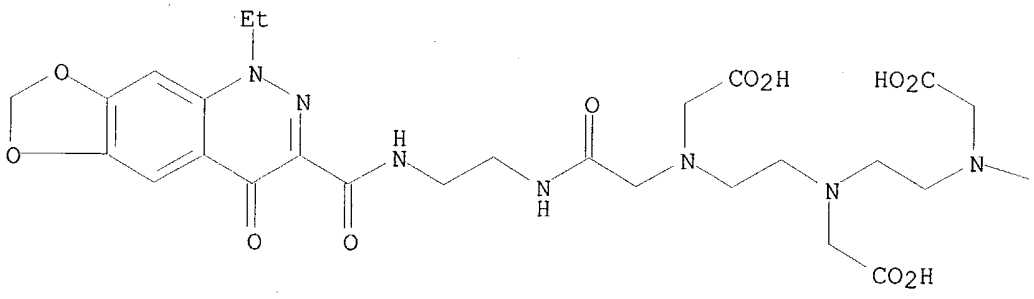
IT **253121-87-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel compds.)

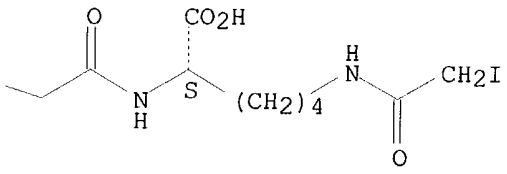
RN 253121-87-8 HCAPLUS

CN L-Lysine, N-[3,6-bis(carboxymethyl)-13-(1-ethyl-1,4-dihydro-4-oxo[1,3]dioxolo[4,5-g]cinnolin-3-yl)-8,13-dioxo-3,6,9,12-tetraazatridec-1-yl]-N-(carboxymethyl)glycyl-N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





L12 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:222922 HCAPLUS
DOCUMENT NUMBER: 130:252610
TITLE: Method for producing cyclohexyl and heterocyclyl nucleoside derivs. and oligomers and their use in pairing or testing systems
INVENTOR(S): Miculka, Christian; Windhab, Norbert; Eschenmoser, Albert; Scherer, Stefan; Quinkert, Gerhard
PATENT ASSIGNEE(S): Aventis Research & Technologies G.m.b.H. & Co. K.-G., Germany
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9915509	A2	19990401	WO 1998-EP6002	19980921
WO 9915509	A3	19990624		
W: AU, BR, CA, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
DE 19741739	A1	19990401	DE 1997-19741739	19970922
CA 2301641	AA	19990401	CA 1998-2301641	19980921
AU 9894412	A1	19990412	AU 1998-94412	19980921
AU 752521	B2	20020919		
BR 9812375	A	20000919	BR 1998-12375	19980921
EP 1049678	A2	20001108	EP 1998-947540	19980921
R: AT, CH, DE, FR, GB, IT, LI, NL				
JP 2001517659	T2	20011009	JP 2000-512817	19980921
US 6689884	B1	20040210	US 2000-509040	20000803

PRIORITY APPLN. INFO.: DE 1997-19741739 A 19970922
WO 1998-EP6002 W 19980921
OTHER SOURCE(S): MARPAT 130:252610
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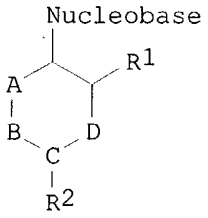


I

AB The invention relates to a compound of formula (I), wherein R1 is NR3R4, OR3 or SR3 with R3 and R4 being H or CnH2n+1 independently of each other and being the same or different, n being a whole number from 1 to 12; R2 is equal to CmH2m-C(X)-Y with X being =O, =S or =N, Y being equal to OR3, NR3R4 or SR3, R3 and R4 having the same meaning given above, and m being a whole number from 1 to 4; or R2 is equal to CmH2m-Z-Y' with Z being a sulfonyl, phosphonyl, ether or amine group, Y' being equal to H, CnH2n+1, OR3, NR3R4 or SR3 then Z is sulfonyl or phosphonyl group, n, R3 and R4 having the meaning given above, and Y' being equal to CnH2n+1 when Z is an ether or an amine group; A, B, and D are the same or different and mean CR5R6, O, NR7 or S independently of each other with R5, R6 and R7 being H or CnH2n+1, independently of each other, n having the meaning given above; and C is equal to CR8 or N with R8 having the meaning of R5 independently, A-B, B-C or C-D not being two identical hetero-atoms; and nucleobase means thymine, uracil, adenine, cytosine, guanine, iso-cytosine, iso-guanine, xanthine or hypoxanthine. The invention also relates to a method for producing these derivs. and to their use in pairing and/or testing systems. These compds. are of interest because they form the building units of cyclohexylnucleooligoamides (CNAs), which have the ability to base-pair with natural DNAs or RNAs, without the steric considerations posed by the ribo- or deoxy-ribo-furan rings of natural (deoxy)nucleic acids. Thus, (S,S,S)-2-iodo-8-aza[3.3.1]nonan-7-one was reacted with 3-(benzyloxy)methyl-thymine, to yield, after a series of protection/deprotection steps, I [A, B, D = CH2; C = (S)-CH; Nucleobase = thymine; R1 = (S)-BOC-NH; R2 = (S)-CH2CO2H (II)]. Using II and the adenine-base equivalent, CNAs up to hexamers were synthesized using solid-phase techniques, and their self-complimentary base-pairing strength was measured.

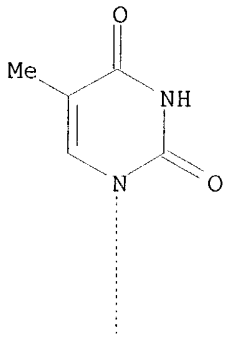
IT **221301-12-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction of in the synthesis of cyclohexyl- and heterocyclyl-nucleoside derivs. and their oligomers or conjugates)

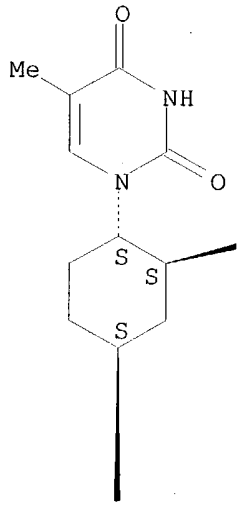
RN 221301-12-8 HCAPLUS

CN L-Lysine, N2-[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-(acetylamino)-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-[3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl]cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-[3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl]cyclohexyl]acetyl]-N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





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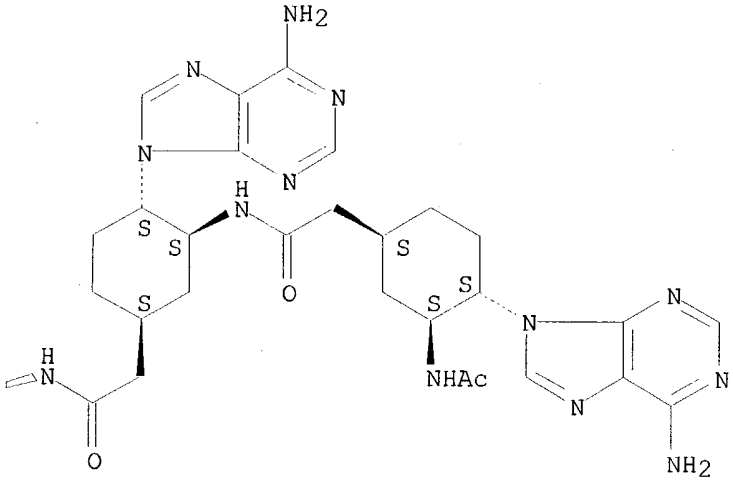
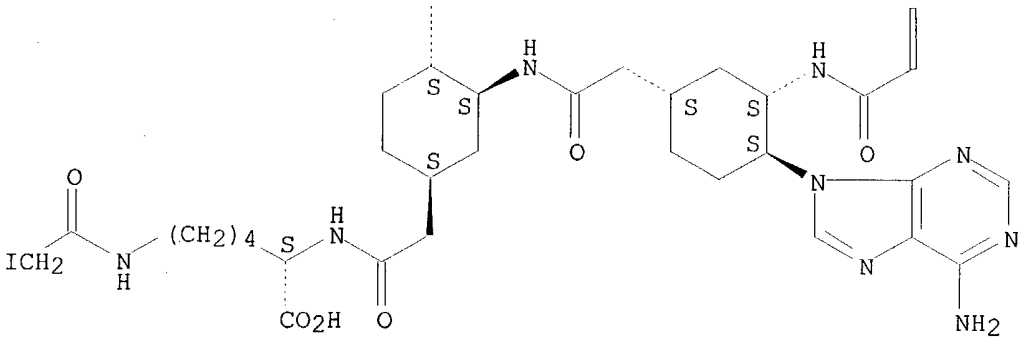


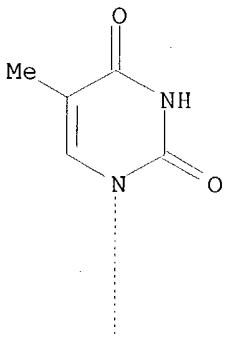
PAGE 2-A



IT **221301-24-2P 221301-36-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(reaction of in the synthesis of cyclohexyl- and heterocyclyl-nucleoside derivs. and their oligomers or conjugates)
RN 221301-24-2 HCAPLUS
CN Glycine, N2-[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-(acetylamino)-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]-N6-(iodoacetyl)-L-lysyl-L-cysteinyl-L-seryl-L-lysyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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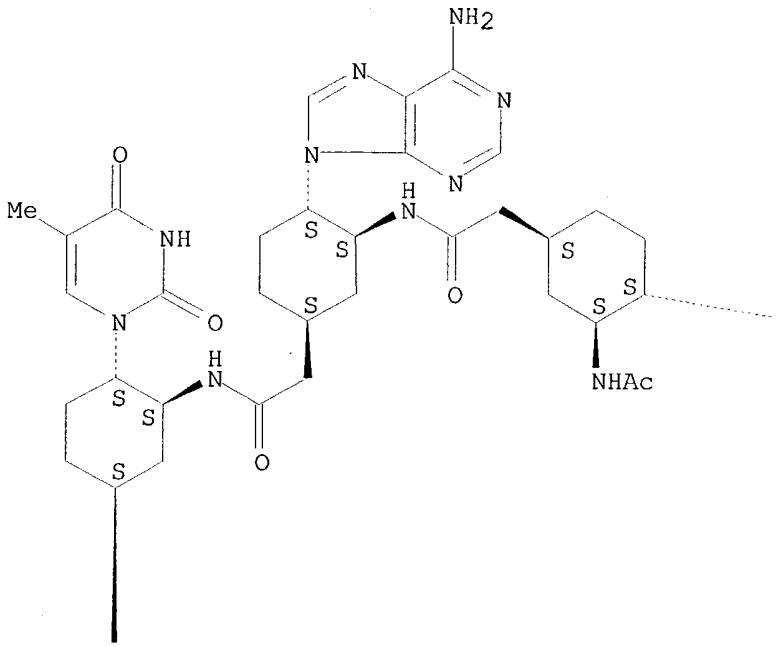
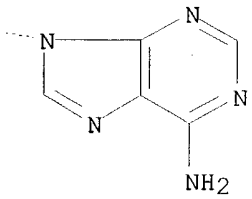


PAGE 1-C



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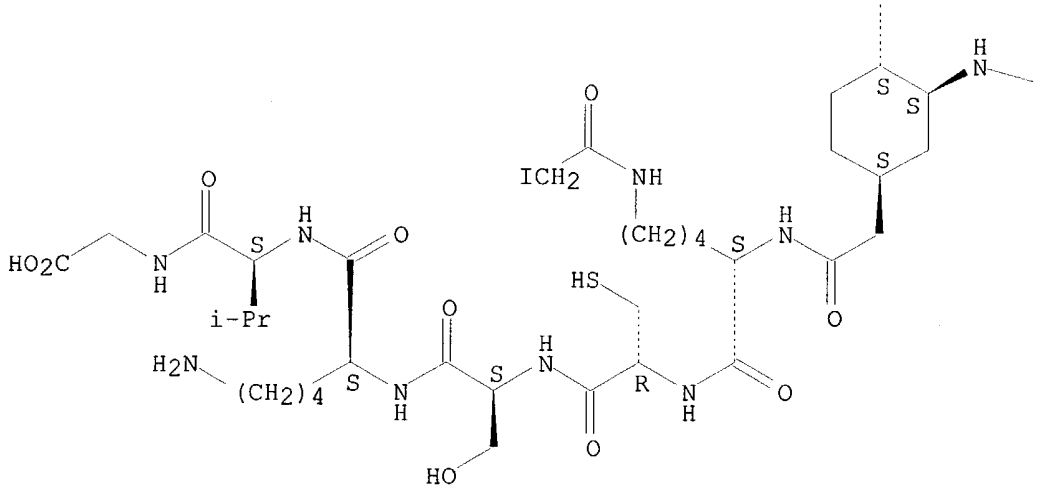
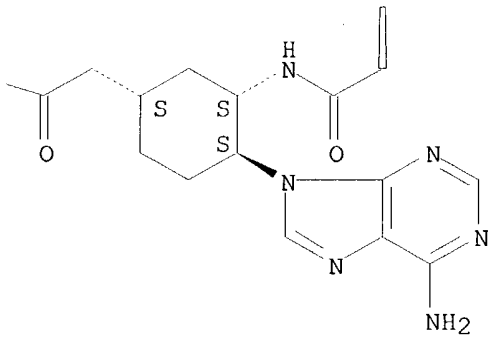


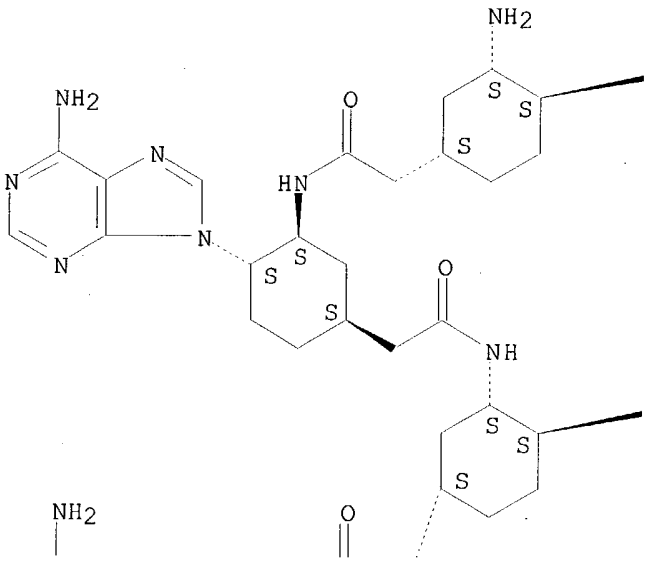
PAGE 2-B



RN 221301-36-6 HCAPLUS
CN Glycine, N2-[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-[[[(1S,3S,4S)-3-amino-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]amino]-4-(6-amino-9H-purin-9-yl)cyclohexyl]acetyl]amino]-4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)cyclohexyl]acetyl]-N6-(iodoacetyl)-L-lysyl-L-cysteinyl-L-tyrosyl-L-seryl-L-lysyl-L-valyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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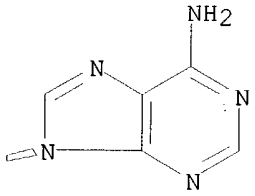

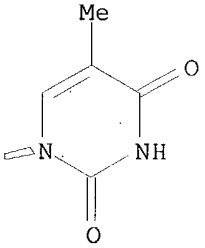

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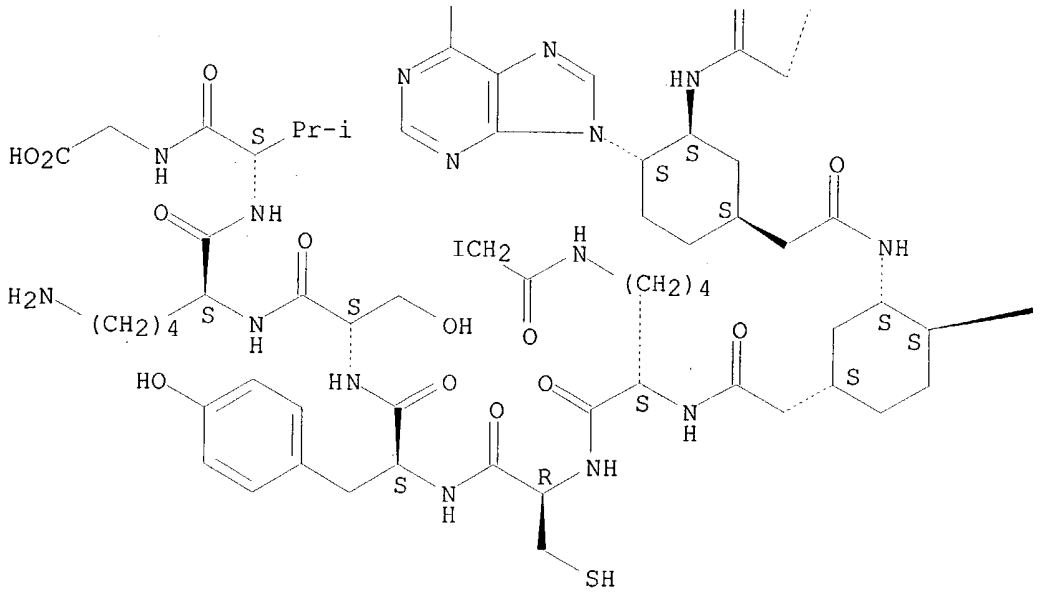

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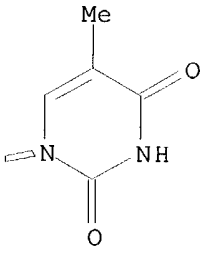


L12 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:27976 HCAPLUS
DOCUMENT NUMBER: 130:89851
TITLE: Automated system for two-dimensional gel electrophoresis analysis of sulfhydryl group-containing proteins
INVENTOR(S): Anderson, N. Leigh; Anderson, Norman G.; Goodman, Jack
PATENT ASSIGNEE(S): Large Scale Biology Corporation, USA
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9859092	A1	19981230	WO 1998-US7387	19980414
W: CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5993627	A	19991130	US 1997-881761	19970624
EP 1003925	A1	20000531	EP 1998-915527	19980414
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002514309	T2	20020514	JP 1999-504390	19980414
US 6136173	A	20001024	US 1999-339165	19990624
US 6391650	B1	20020521	US 1999-339177	19990624
US 6123821	A	20000926	US 1999-405213	19990927
US 2001015320	A1	20010823	US 2001-813321	20010321
US 6482303	B2	20021119		
US 2001032786	A1	20011025	US 2001-851245	20010509
US 2002175078	A1	20021128	US 2002-92848	20020306
US 2002133300	A1	20020919	US 2002-95461	20020313
US 2002157954	A1	20021031	US 2002-95427	20020313

PRIORITY APPLN. INFO.:

US 1997-881761	A	19970624
WO 1998-US7387	W	19980414
US 1999-339164	A1	19990624
US 1999-339165	A3	19990624
US 1999-339177	A3	19990624
US 2000-580266	A1	20000526
US 2000-642246	A3	20000817
US 2000-642247	A3	20000817
US 2000-680443	A1	20001006
US 2001-809143	A1	20010316

AB An integrated, fully automated, high-throughput system for two-dimensional electrophoresis comprised (2-D) of gel-making and gel-casting machines, gel processing machines, gel compns. and geometries, gel handling systems, sample preparation systems, and software, especially for treatment and anal. of protein-containing samples. The method provides for reduction and alkylation of cysteine sulfhydryl group in the samples in order to preserve the isoelec. point of sample proteins and to prevent protein loss in the 2-D process by (for example) protein aggregation or refolding associated with sulfhydryl group re-oxidation The method can prepare IPG (immobilized pH gradient) gels of different cross section for optimization of high-resolution protein sepns.

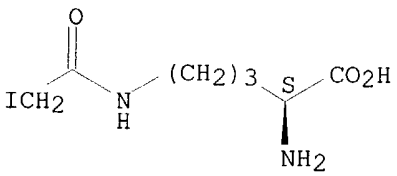
IT **35748-65-3**

RL: ARG (Analytical reagent use); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)
(alkylating agent; in automated system for two-dimensional gel electrophoresis anal. of sulfhydryl group-containing proteins)

RN 35748-65-3 HCAPLUS

CN L-Ornithine, N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

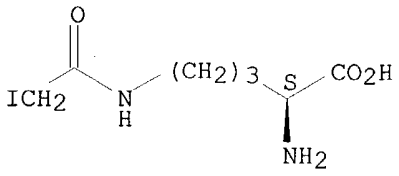
L12 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:11414 HCAPLUS
DOCUMENT NUMBER: 130:192897
TITLE: Modulation of sulfur mustard toxicity by arginine analogs and related nitric oxide synthase inhibitors in vitro
AUTHOR(S): Sawyer, Thomas W.
CORPORATE SOURCE: Therapy Group, Medical Countermeasures Section, Defence Research Establishment Suffield, Medicine Hat, AB, T1A 8K6, Can.
SOURCE: Toxicological Sciences (1998), 46(1), 112-123
CODEN: TOSCF2; ISSN: 1096-6080
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The modulating effects of a series of arginine analogs and related nitric oxide synthase inhibitors against the toxicity of sulfur mustard (HD) in primary cultures of chick embryo forebrain neurons were examined In addition to the previously identified protective compds., D- and L-nitroarginine Me ester, eight addnl. arginine analogs were shown to have significant, concentration-dependent protective characteristics against HD toxicity. Of these, L-nitroarginine was the most potent, increasing the LC50 of vehicle-pretreated HD-treated control cultures by .apprx.350%. In addition to these protective agents, five compds. related to arginine were also identified that potentiated the toxicity of HD in the neuron cultures in a concentration-dependent manner. This action occurred at concns. where these chems. alone exhibited no toxicity. Characterization of the active compds. in this study showed that it was likely that the protective agents, as well as those compds. that potentiated HD toxicity, were exerting their effects at the same biochem. target, but not through the inhibition of nitric oxide synthase. Although the identity of this target site is as yet unknown, these studies demonstrate that subtle alterations to the arginine structure can yield compds. that differentially modulate the toxicity of HD through their activity at a common target site. (c) 1998 Society of Toxicology.

IT **35748-65-3 90764-56-0**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(modulation of sulfur mustard toxicity by arginine analogs in relation to nitric oxide synthase)

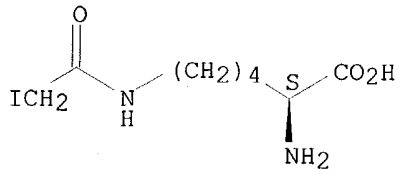
RN 35748-65-3 HCAPLUS
CN L-Ornithine, N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 90764-56-0 HCAPLUS
CN L-Lysine, N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



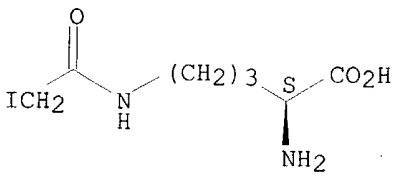
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:292185 HCAPLUS
DOCUMENT NUMBER: 124:333347
TITLE: Antifertility effects of (+)-S-2-amino-6-iodoacetamidohexanoic acid (2-AIHA) in female rats
AUTHOR(S): Chamorro, German; Salazar, Maria; Salazar, Silvia; Ceballos, Guillermo; Trujillo, Jose; Munoz, Olga; Yanez, Ricardo
CORPORATE SOURCE: Department Toxicology, National School Biological Sciences, Mexico City, 11591, Mex.
SOURCE: Contraception (1996), 53(4), 247-251
CODEN: CCPTAY; ISSN: 0010-7824
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB (+)-S-2-amino-6-iodoacetamidohexanoic acid (AIHA), an irreversible inhibitor of the ornithine decarboxylase and extrahepatic arginase enzymic activities with antineoplastic properties, was evaluated for antifertility activity in pregnant rats by oral administration at different periods of gestation. Our results showed that doses of 10 and 20 mg/kg of AIHA orally administered produced a contraceptive effect when it was administered from days 2 to 5, and 8 to 12 of gestation, resp. The gestation time was slightly shortened when AIHA was applied from day 15 until labor. No sign of external malformations in fetuses was observed AIHA did not affect the total length of estrous cycle at the same dosage level used to interrupt pregnancy. In ovariectomized immature rats, neither changes in uterine weight, premature vaginal opening, or cornified cells were found. However, AIHA enhanced the estradiol-induced increase in uterine weight when both were concomitantly administered.

IT **35748-65-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antifertility effects of aminoiodoacetamidohexanoic acid in female)
RN 35748-65-3 HCAPLUS
CN L-Ornithine, N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

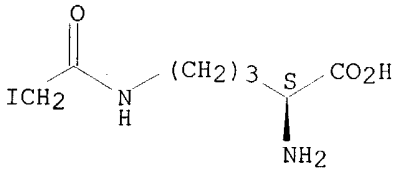
ACCESSION NUMBER: 1993:93945 HCAPLUS
DOCUMENT NUMBER: 118:93945
TITLE: Antitumor effect and toxicity of two new active-site-directed irreversible ornithine decarboxylase and extrahepatic arginase inhibitors
AUTHOR(S): Trujillo-Ferrara, Jose; Koizumi, Guadalupe; Munoz, Olga; Joseph-Nathan, Pedro; Yanez, Ricardo
CORPORATE SOURCE: Esc. Super. Med., Inst. Politec. Nac., Mexico City, 11340, Mex.
SOURCE: Cancer Letters (Shannon, Ireland) (1992), 67(2-3), 193-7
CODEN: CALEDQ; ISSN: 0304-3835
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The irreversible ornithine decarboxylase and extrahepatic arginase inhibitors (+)-S-2-amino-5-iodoacetamidopentanoic acid (2-AIPA) and (+)-S-2-amino-6-iodoacetamido-hexanoic acid (2-AIHA) were evaluated. The LD50 tests were made in rats and mice using both compds. Rats and mice were treated with either 2-AIPA or 2-AIHA i.p. for a period of 180 days. The treated animals showed a decrease of total serum proteins and increased ALT and AST levels. CK was also modified but inversely related to dose. Protection tests were carried out using L5178Y mouse lymphosarcoma. The mean survival time for each treated group was calculated and the percentage T/C was determined For 2-AIPA it was 170 and for 2-AIHA it was 210 at 15 mg/kg.

IT **35748-65-3 90764-56-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antitumor activity of, as polyamine biosynthesis inhibitor)

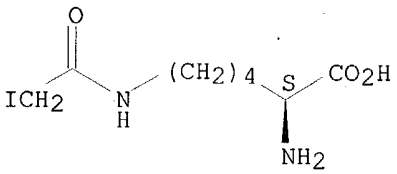
RN 35748-65-3 HCAPLUS
CN L-Ornithine, N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 90764-56-0 HCAPLUS
CN L-Lysine, N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:515042 HCAPLUS
DOCUMENT NUMBER: 115:115042

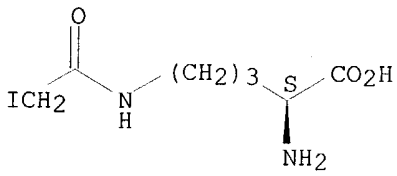
TITLE: Regioselective synthesis of (+)-(S)-2-amino-5-(iodoacetamido)pentanoic and (+)-(S)-2-amino-6-(iodoacetamido)hexanoic acids
AUTHOR(S): Trujillo, J. G.; Ceballos, G.; Yanez, R.; Joseph-Nathan, P.
CORPORATE SOURCE: Esc. Super. Med., Inst. Politec. Nac., Mexico City, Mex.
SOURCE: Synthetic Communications (1991), 21(5), 683-91
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:115042

AB Title amino acids ICH2CONH(CH2)nCH(NH2)CO2H (n = 3, 4) were prepared by acylation of ornithine or lysine in aqueous THF. The 13C chemical shifts of the products were recorded as a function of solution pH.

IT **35748-65-3P 90764-56-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and carbon-13 NMR of)

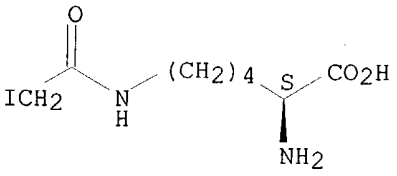
RN 35748-65-3 HCAPLUS
CN L-Ornithine, N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 90764-56-0 HCAPLUS
CN L-Lysine, N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



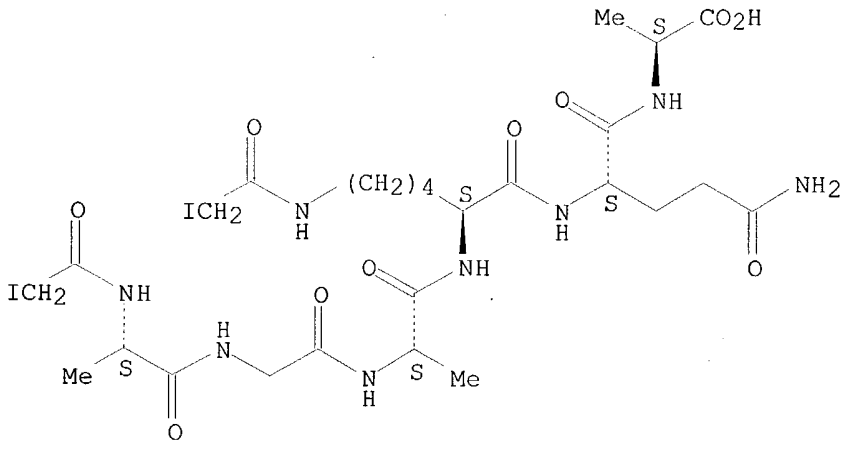
L12 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:175189 HCAPLUS
DOCUMENT NUMBER: 112:175189
TITLE: A general method for highly selective crosslinking of unprotected polypeptides via pH-controlled modification of N-terminal α-amino groups
AUTHOR(S): Wetzel, Ronald; Halualani, Roger; Stults, John T.; Quan, Clifford
CORPORATE SOURCE: Dep. Protein Chem., Genentech, Inc., San Francisco, CA, 94080, USA
SOURCE: Bioconjugate Chemistry (1990), 1(2), 114-22
CODEN: BCCHES; ISSN: 1043-1802
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A method is described for the highly selective modification of the α-NH2 groups at the N-termini of unprotected peptides to form stable, modified peptide intermediates that can be covalently coupled to other mols. or to a solid support. Acylation with iodoacetic anhydride at pH 6.0 occurs with 90-98% selectivity for the α-NH2 group, depending on the N-terminal residue (as shown with a series of model hexapeptides containing a competing lysine residue). Although cysteine residues must be protected (reversibly or irreversibly) before the anhydride reaction, there are no detectable side reactions of the α-NH2 moiety (of the reagent or of modified peptide) with the side chains of histidine, methionine, or lysine. The reaction works well in denaturants so that inhibitory effects of noncovalent structure can be minimized. In a 2nd step, the iodoacetyl-peptide can be reacted with a thiol group on a protein, on a solid chromatog. matrix, on a spectroscopic probe, etc. This is illustrated by reaction of a series of Nα-iodoacetyl-peptides with murine interferon-γ, which contains a C-terminal cysteine residue. The iodoacetic anhydride scheme is superior in selectivity for α-NH2 groups to conventional chemical approaches to crosslinking and the reaction is suited for modifying peptide fragments, as pure species or as mixts., derived from proteolytic or chemical fragmentation of proteins. Peptides synthesized biosynthetically, e.g., via recombinant DNA techniques, can be crosslinked in this way. It may be possible to crosslink small amts. of proteinaceous biol. factors and, thus, develop affinity matrixes or make antibodies before the polypeptide of interest has been fully purified or structurally characterized.

IT **125713-55-5P 125713-56-6P 125713-57-7P**
125713-58-8P 125713-59-9P 125713-60-2P
125713-61-3P 125713-62-4P 125713-63-5P
125713-64-6P 125713-65-7P 125713-66-8P
125713-67-9P 125713-68-0P 125713-69-1P
125713-70-4P 125713-71-5P 125713-72-6P
125713-73-7P 125713-74-8P
RL: PREP (Preparation)
(preparation of, peptide crosslinking in relation to)

RN 125713-55-5 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-alanyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

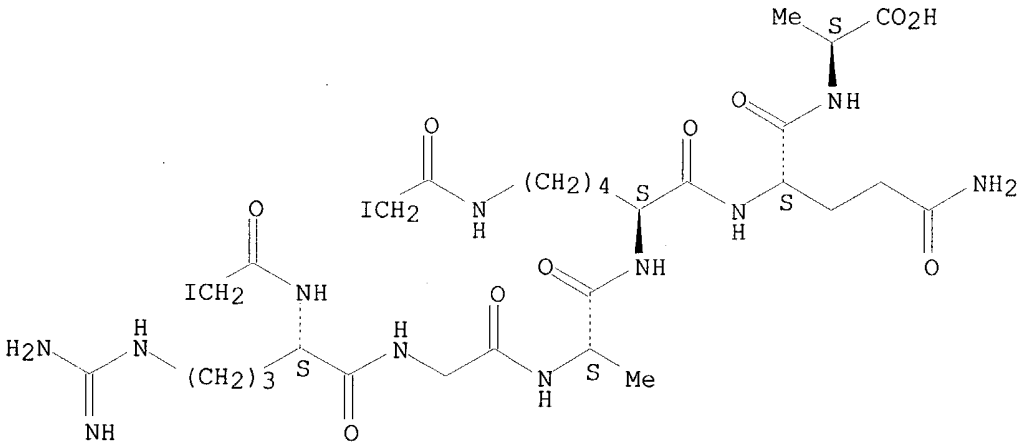
Absolute stereochemistry.



RN 125713-56-6 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N2-(iodoacetyl)-L-

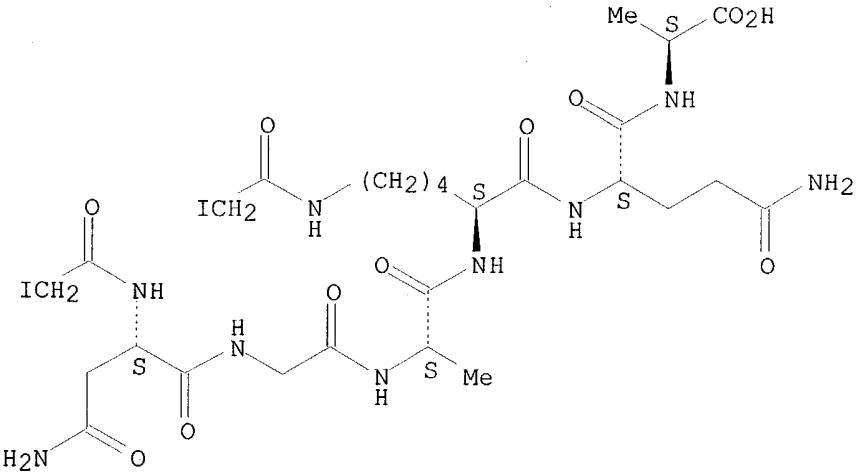
arginyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



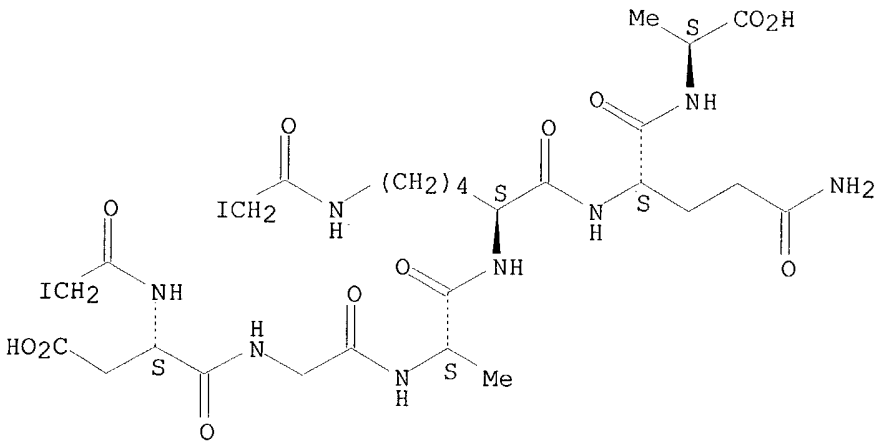
RN 125713-57-7 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N2-(iodoacetyl)-L-asparaginyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 125713-58-8 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-α-aspartyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

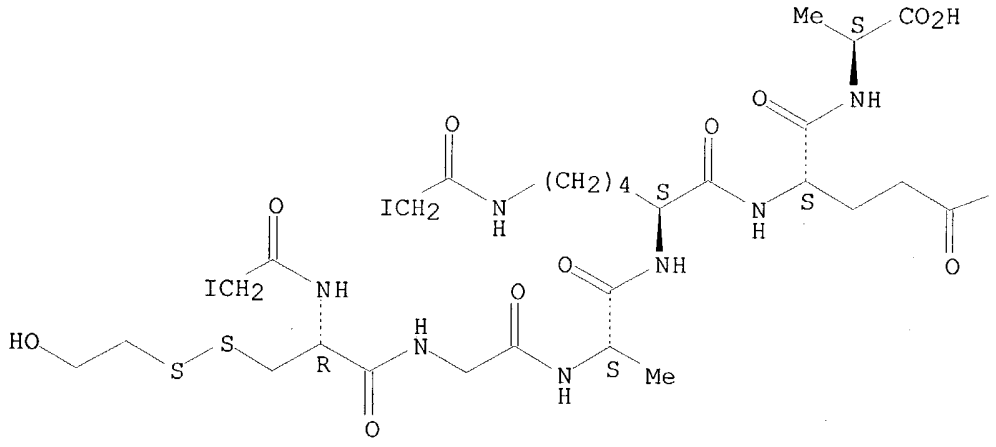
Absolute stereochemistry.



RN 125713-59-9 HCAPLUS
CN L-Alanine, N-[N2-[N2-[N-[N-[3-[(2-hydroxyethyl)dithio]-N-(iodoacetyl)-L-alanyl]glycyl]-L-alanyl]-N6-(iodoacetyl)-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

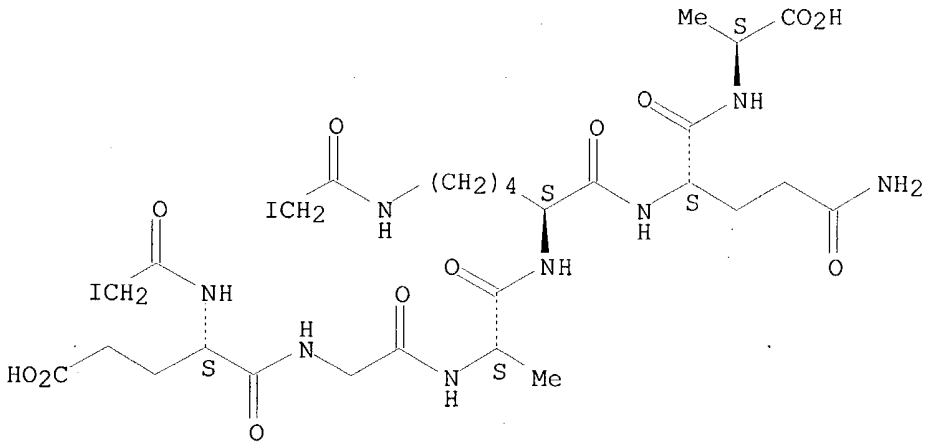


PAGE 1-B

RN 125713-60-2 HCAPLUS

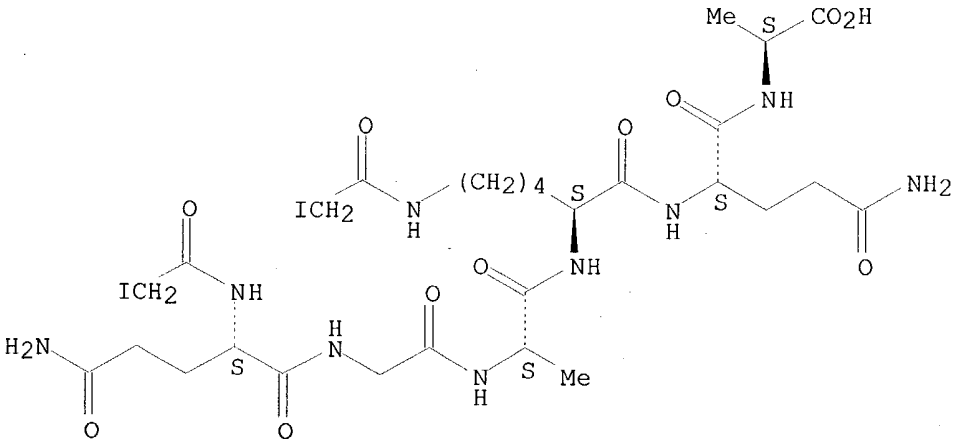
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-α-glutamyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



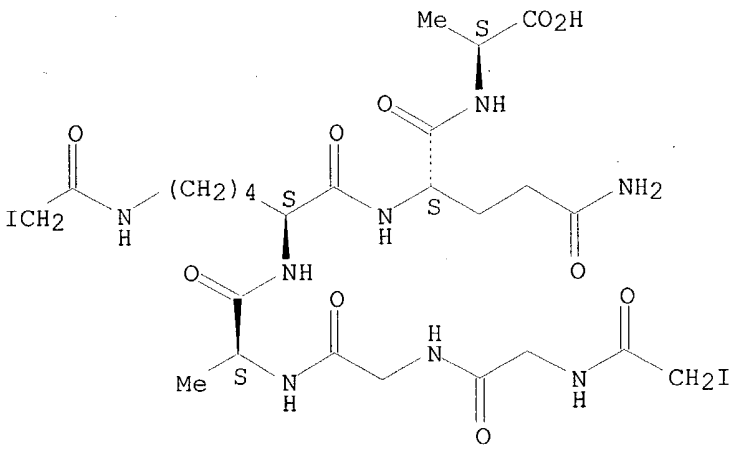
RN 125713-61-3 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N2-(iodoacetyl)-L-glutaminyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



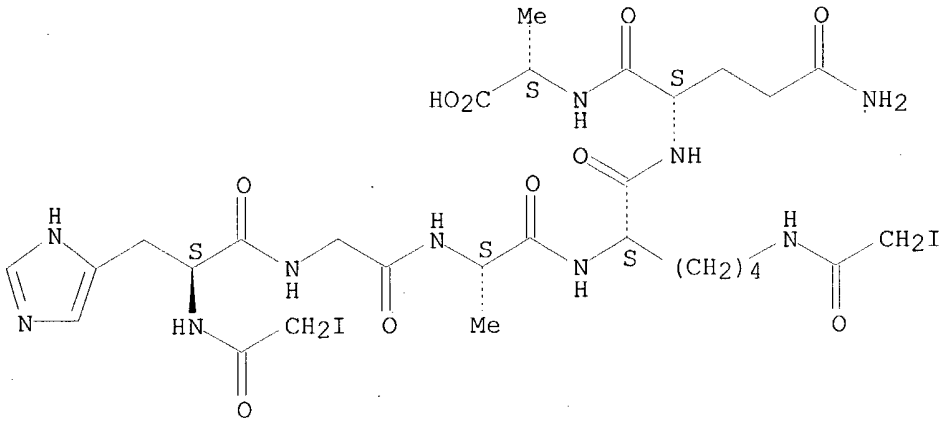
RN 125713-62-4 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)glycyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



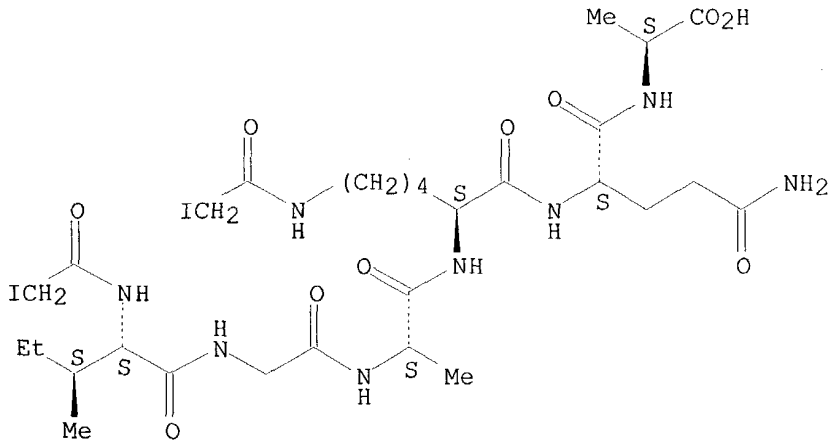
RN 125713-63-5 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-histidyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



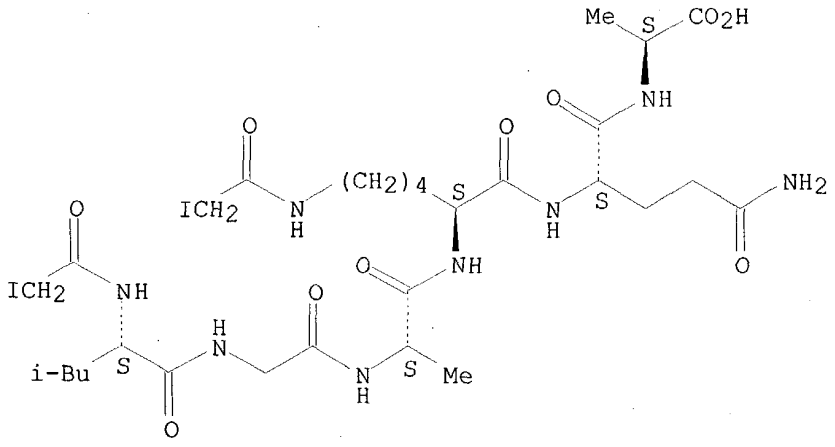
RN 125713-64-6 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-isoleucyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



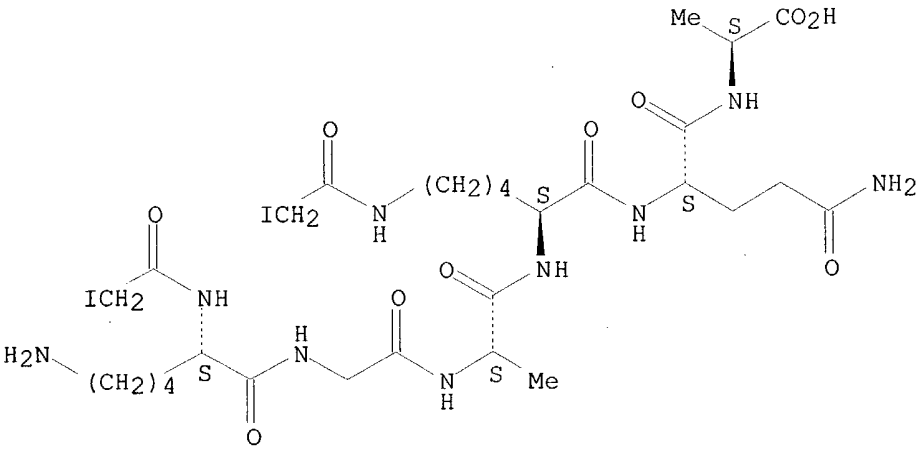
RN 125713-65-7 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-leucyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



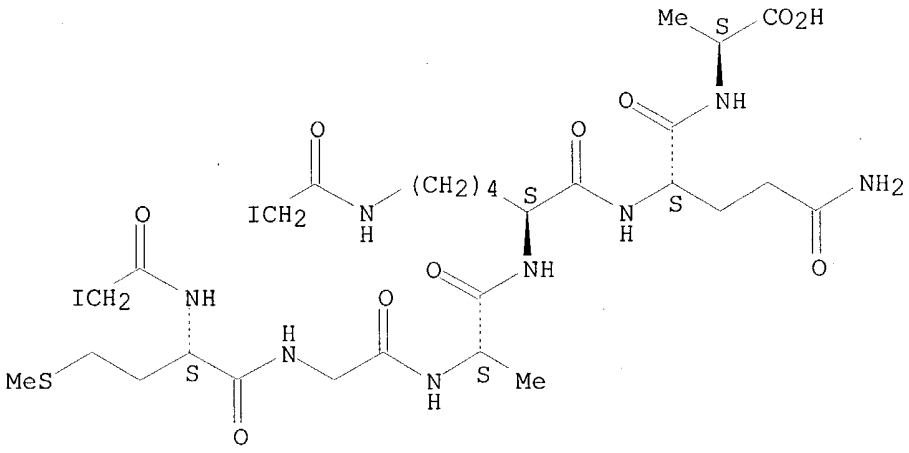
RN 125713-66-8 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N2-(iodoacetyl)-L-lysyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



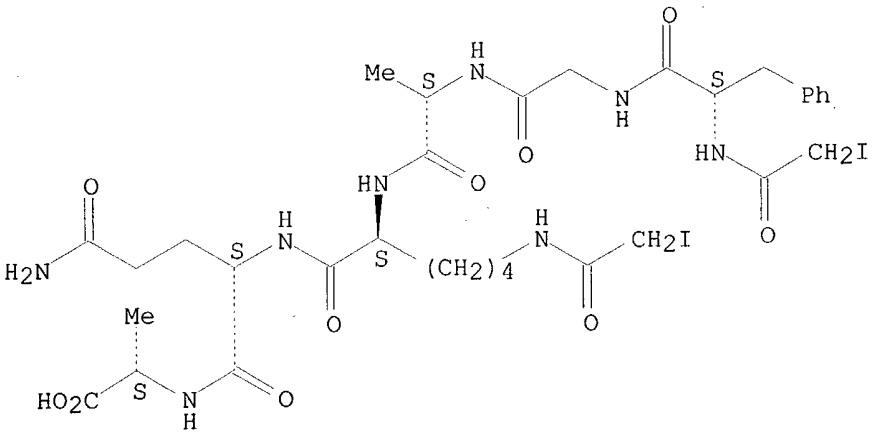
RN 125713-67-9 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-methionyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



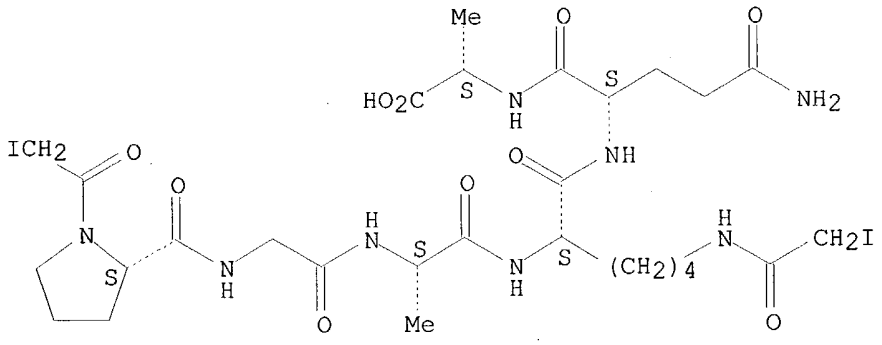
RN 125713-68-0 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-phenylalanyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



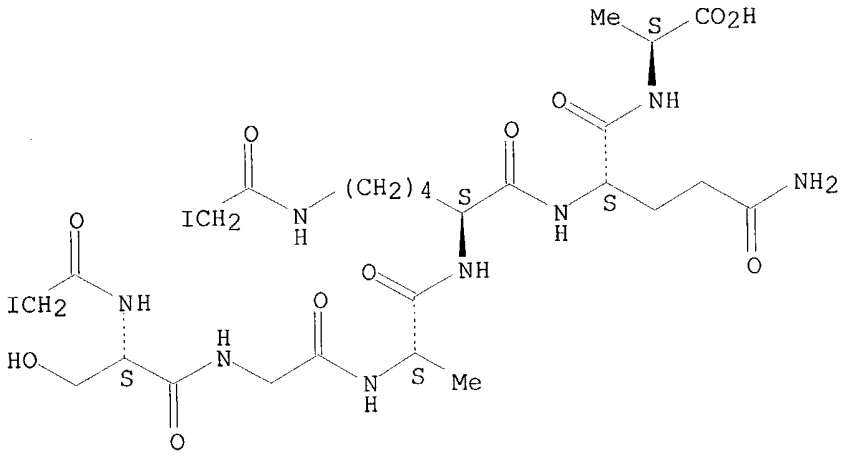
RN 125713-69-1 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[1-(iodoacetyl)-L-prolyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



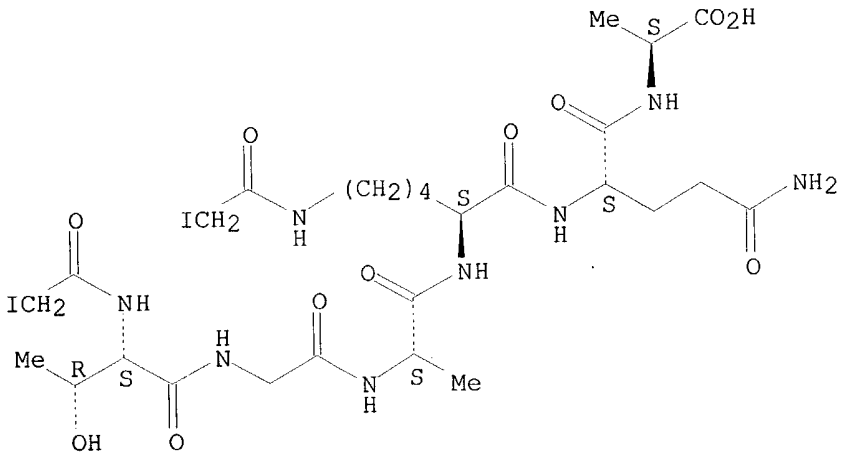
RN 125713-70-4 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-seryl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 125713-71-5 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-threonyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

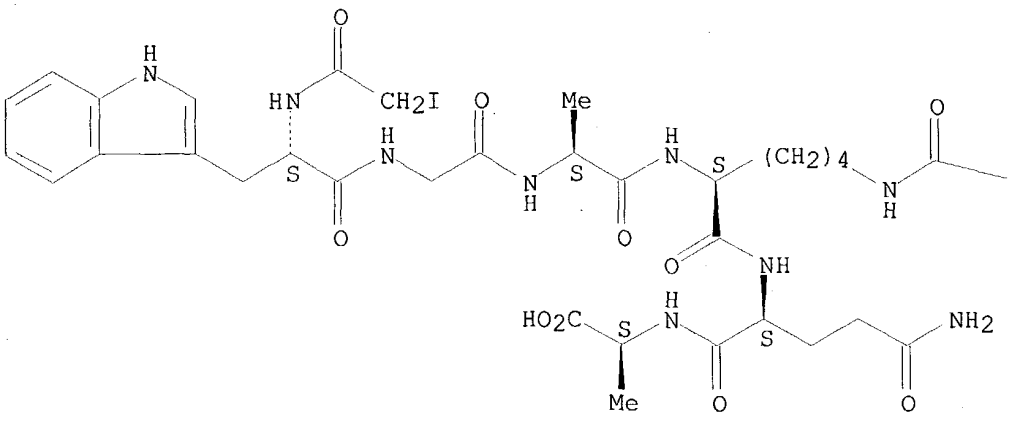
Absolute stereochemistry.



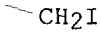
RN 125713-72-6 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-tryptophyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

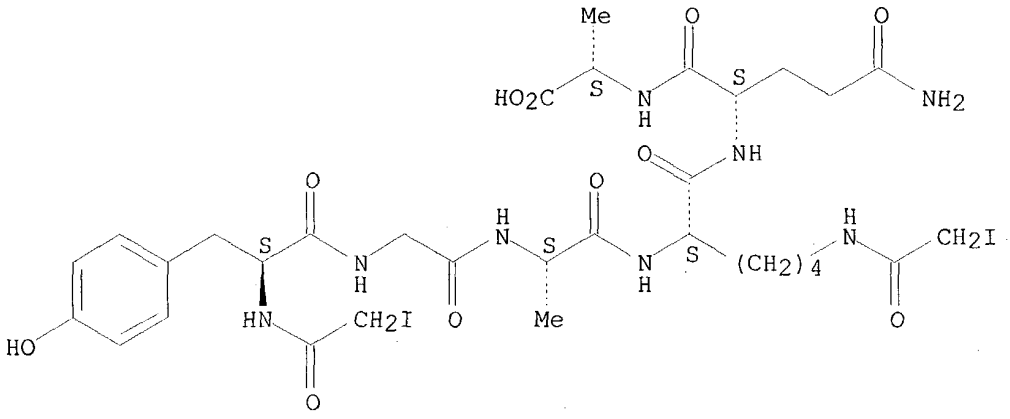


PAGE 1-B



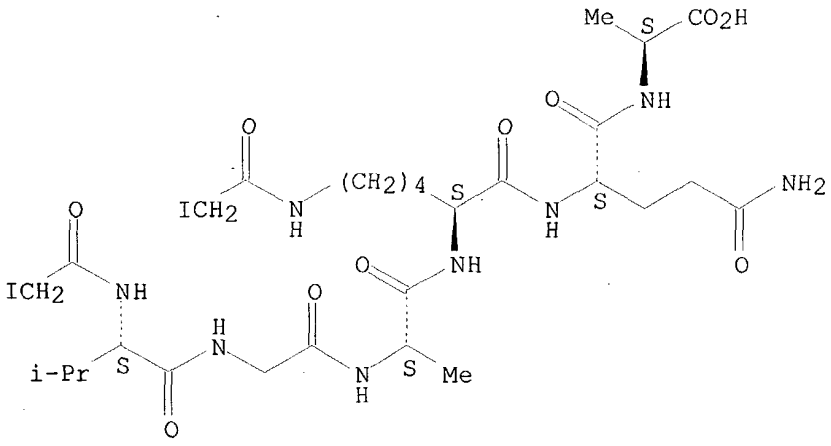
RN 125713-73-7 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-tyrosyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

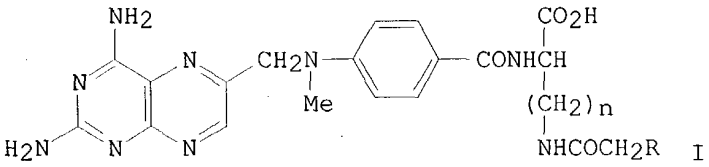


RN 125713-74-8 HCAPLUS
CN L-Alanine, N-[N2-[N6-(iodoacetyl)-N2-[N-[N-[N-(iodoacetyl)-L-valyl]glycyl]-L-alanyl]-L-lysyl]-L-glutaminyl]- (9CI) (CA INDEX NAME)

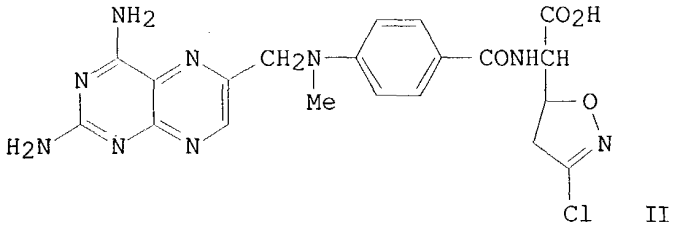
Absolute stereochemistry.



L12 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:470356 HCAPLUS
DOCUMENT NUMBER: 107:70356
TITLE: Methotrexate analogs. 30. Dihydrofolate reductase inhibition and in vitro tumor cell growth inhibition by Nε-(haloacetyl)-L-lysine and Nδ-(haloacetyl)-L-ornithine analogs and an acivicin analog of methotrexate
AUTHOR(S): Rosowsky, Andre; Solan, Vishnu C.; Forsch, Ronald A.; Delcamp, Tavner J.; Baccanari, David P.; Freisheim, James H.
CORPORATE SOURCE: Dana-Farber Cancer Inst., Harvard Med. Sch., Boston, MA, 02115, USA
SOURCE: Journal of Medicinal Chemistry (1987), 30(8), 1463-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



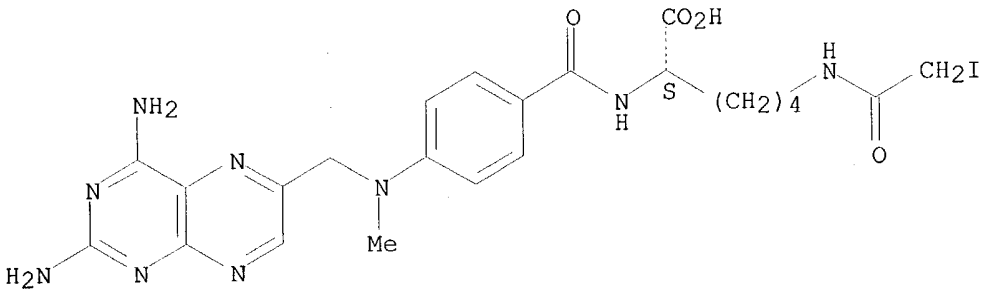
II

AB Analogs of methotrexate (MTX) ((I; R = Br, Cl, or I; n = 3 or 4) and II)

with strong alkylating activity were prepared by replacing and L-glutamate side chain with Nω-haloacetyl derivs. of L-lysine and L-ornithine. Haloacetylation was accomplished in 30-40% yield by reaction of the preformed L-lysine and L-ornithine analogs of MTX with p-nitrophenyl bromoacetate or chloroacetate in aqueous NaHCO3 at room temperature All 4 haloacetamides were potent inhibitors in spectrophotometric assays measuring noncovalent binding to purified dihydrofolate reductase (DHFR) from L1210 cells. In expts. designed to measure time-dependent inactivation of DHFR from L1210 cells and Candida albicans, and Nε-(bromoacetyl)-L-lysine and Nδ-(bromoacetyl)-L-ornithine analogs gave results consistent with covalent binding, whereas Nε- and Nv-chloroacetyl analogs did not. The Nv-(bromoacetyl)-L-ornithine analog appeared to be the more reactive one toward both enzymes. Amino acid anal. of acid hydrolyzates of the L1210 enzyme following incubation with the bromoacetamides failed to demonstrate the presence of a carboxymethylated residue, suggesting that alkylation had perhaps formed an acid-labile bond. In growth inhibition assays with L1210 cultured murine leukemia cells, the 4 haloacetamides were all more potent than their nonacetylated precursors but less potent than MTX. The >40000-fold MTX-resistant mutant cell line L1210/R81 was only partly cross-resistant to the haloacetamides. An analog of MTX with acivicin replacing glutamate was a potent inhibitor of DHFR from chicken liver and L1210 cells but was 200 times less potent than MTX against L1210 cells in culture.

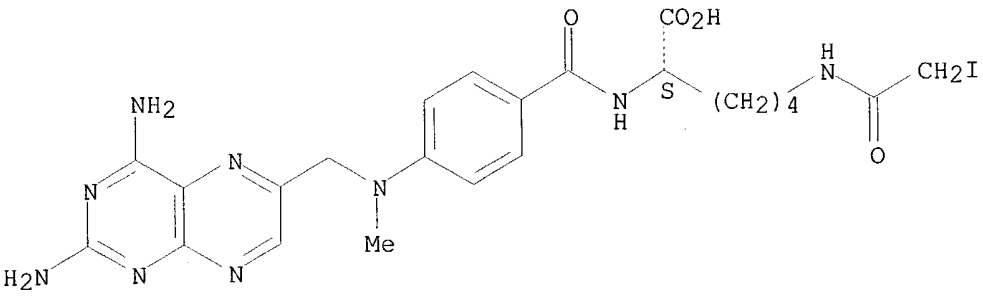
IT **82339-36-4**
RL: BIOL (Biological study)
(antitumor and dihydrofolate reductase-inhibiting activity of)
RN 82339-36-4 HCAPLUS
CN L-Lysine, N2-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **108743-13-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antitumor and dihydrofolate reductase-inhibiting activity of)
RN 108743-13-1 HCAPLUS
CN L-Lysine, N2-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-N6-(iodoacetyl)-, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Na

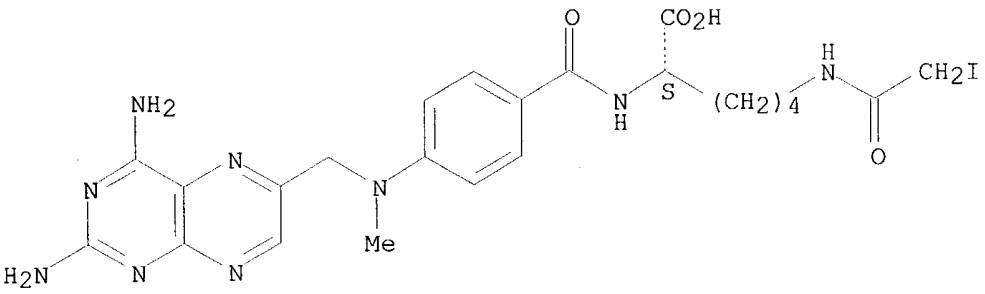
L12 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:29310 HCAPLUS
DOCUMENT NUMBER: 106:29310
TITLE: Affinity labeling of dihydrofolate reductase with an iodoacetyl lysine analog of methotrexate
AUTHOR(S): Delcamp, T. J.; Rosowsky, A.; Smith, P. L.; Wright, J. E.; Freisheim, J. H.
CORPORATE SOURCE: Dep. Biochem., Med. Coll. Ohio, Toledo, OH, 43699, USA
SOURCE: Chem. Biol. Pteridines, 1986, Pteridines Folic Acid Deriv., Proc. Int. Symp. Pteridines Folic Acid Deriv.: Chem., Biol. Clin. Aspects, 8th (1986), 807-9. Editor(s): Cooper, Bernard A.; Whitehead, V. Michael. de Gruyter: Berlin, Fed. Rep. Ger.
CODEN: 55HGAH
DOCUMENT TYPE: Conference
LANGUAGE: English

AB The covalent labeling of dihydrofolate reductases (I) from Lactobacillus casei, chicken liver, and a methotrexate-resistant human lymphoblastoid cell line with Nα-(4-amino-4-deoxy-N10-methylpteroyl)-Nε-(iodoacetyl)-L-lysine (II) is described. Each of the 3 I enzymes was competitively inhibited by II, indicating an initial binding of the compound Sequence anal. of modified bacterial I demonstrated that histidine-28 was the residue modified by II. In human and chicken liver I, the single cysteine (Cys) of each enzyme (Cys-6 and Cys-11, resp.) were the residues modified by II. Thus, II can react covalently with I from 3 different sources with noteworthy differences in the sites of modification.

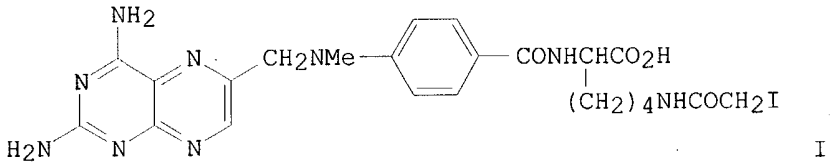
IT **82339-36-4**
RL: BIOL (Biological study)
(dehydrofolate reductase of human and other sources affinity labeling with, different sites of)

RN 82339-36-4 HCAPLUS
CN L-Lysine, N2-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:449316 HCAPLUS
DOCUMENT NUMBER: 97:49316
TITLE: Methotrexate analogs. 15. A methotrexate analogue designed for active-site-directed irreversible inactivation of dihydrofolate reductase
AUTHOR(S): Rosowsky, A.; Wright, J. E.; Ginty, C.; Uren, J.
CORPORATE SOURCE: Sidney Farber Cancer Inst., Harvard Med. Sch., Boston, MA, 02115, USA
SOURCE: Journal of Medicinal Chemistry (1982), 25(8), 960-4
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



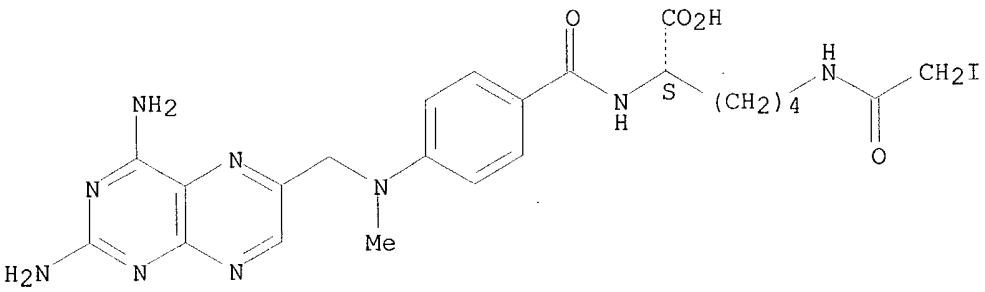
I

AB Nα-(4-amino-4-deoxy-N10-methylpteroyl)-Nε-(iodoacetyl)-L-lysine (I) [**82339-36-4**] was synthesized as a potential active-site-directed irreversible inhibitor of dihydrofolate reductase (EC 1.5.1.3) (DHFR) [9002-03-3]. In an UV spectrophotometric assay of dihydrofolate reduction by Lactobacillus casei DHFR, I and methotrexate had ID50 values of 4.5 and 6.2 nM, resp. The corresponding ID50 values in a competitive radioligand binding assay against [3H]MTX were 31 and 16 nM, resp. Thus, as reversible inhibitors of this enzyme over a short exposure time, I and MTX had comparable activity. On the other hand, when L. casei DHFR was incubated for up to 6 h with 0.1 or 1.0 μM I, a progressive decrease in the ability of [3H]MTX to subsequently displace the drug was observed When MTX itself was used at the same concns., the extent of displacement of [3H]MTX did not decrease with time. These results were consistent with rapid reversible binding of I to the enzyme, followed more slowly by covalent bond formation near the active site. The pH profile for this effect followed a curve with a sigmoidal shape. The apparent inflection point near pH 7.2 was consistent with alkylation of a histidine residue.

IT **82339-36-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dihydrofolate reductase-inhibiting activity of)

RN 82339-36-4 HCAPLUS
CN L-Lysine, N2-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

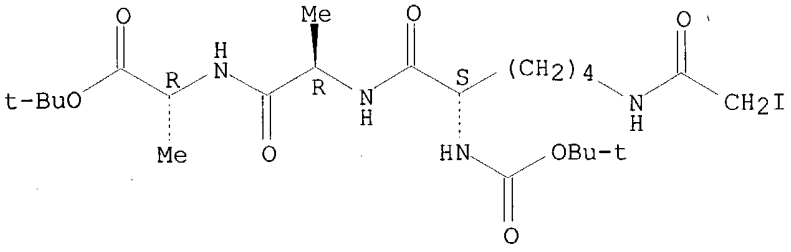


L12 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:562104 HCAPLUS
DOCUMENT NUMBER: 87:162104
TITLE: Antibacterial halogenoacetyl derivatives of amino acids and simple peptides
AUTHOR(S): Goodacre, Jennifer; Jeffries, Leonard; Nayler, John H. C.; Ponsford, Roger J.; Stirling, Irene
CORPORATE SOURCE: Res. Div., Beecham Pharm., Betchworth/Surrey, UK
SOURCE: Journal of Medicinal Chemistry (1977), 20(11), 1445-8
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Protected peptide esters prepared by a standard coupling technique using dicyclohexylcarbodiimide in CH2Cl2 were deprotected, acylated with iodoacetic acid [64-69-7] or bromoacetic acid [79-08-3], and the haloacetyl esters treated with F3CCO2H to give the free acids. None of the 14 free acids had significant activity in vitro against Staphylococcus aureus or Escherichia coli, while several of the 24 haloacetylamino acid esters and haloacetylpeptide esters had appreciable activity, especially against S. aureus. The most active compds., ICH2C(:O)-Gly-Gly-OCH2Ph [63984-36-1], ICH2C(:O)NH(CH2)4CO2CH2Ph [63984-37-2], ICH2C(:O)NH(CH2)4CO2Me [63984-38-3], and ICH2C(:O)NH(CH2)5CO2CH2Ph [63984-39-4] are simple, nonchiral chains. Structure-activity relations and antibacterial mechanisms are discussed.

IT **63984-17-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and bactericidal activity of)
RN 63984-17-8 HCAPLUS
CN D-Alanine, N-[N-[N2-[(1,1-dimethylethoxy)carbonyl]-N6-(iodoacetyl)-L-lysyl]-D-alanyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

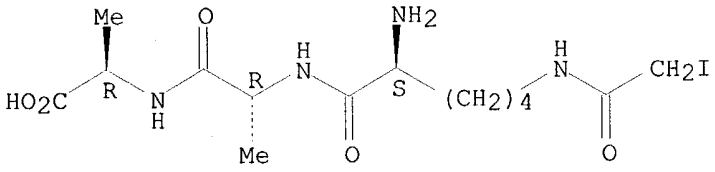


IT **63984-34-9P**
RL: PREP (Preparation)
(preparation of, as bactericide)
RN 63984-34-9 HCAPLUS
CN D-Alanine, N-[N-[N6-(iodoacetyl)-L-lysyl]-D-alanyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

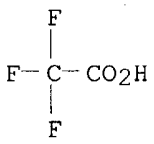
CRN 63984-33-8
CMF C14 H25 I N4 O5

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



L12 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:100013 HCAPLUS
DOCUMENT NUMBER: 76:100013
TITLE: Synthesis of δ-N-haloacetyl ornithine derivatives
AUTHOR(S): Olomucki, Martin; Hebrard, Paul; Le Gall, Jean Y.
CORPORATE SOURCE: Lab. Biochim. Gen. Comp., Coll. France, Paris, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1971), (12), 4524-5
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal

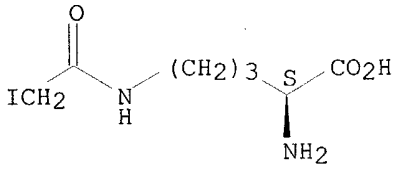
LANGUAGE: French

AB Cu complexes of ornithine hydrochloride, prepared with Cu carbonate, were acylated with p-nitrophenyl haloacetates and demetalation was effected on a Chelex 100 Column. Prepared were L and DL isomers of XCH2C(O)NH(CH2)3CH(NH2)CO2H (X = Br, Cl, iodine).

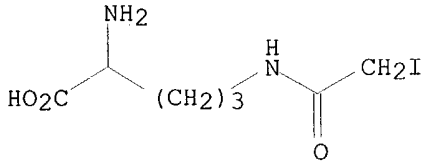
IT **35748-65-3P 35748-66-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 35748-65-3 HCAPLUS
CN L-Ornithine, N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 35748-66-4 HCAPLUS
CN Ornithine, N5-(iodoacetyl)- (9CI) (CA INDEX NAME)

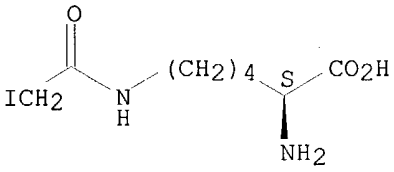


=> □
L13 ANSWER 1 OF 1 CAOLD COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: CA60:10989c CAOLD
TITLE: substrate specificity of the bacterial ε-lysine acylase
AUTHOR NAME: Chibata, Ichiro; Tosa, T.; Ishikawa, T.

=> d hitstr

L13 ANSWER 1 OF 1 CAOLD COPYRIGHT 2004 ACS on STN
IT **90764-56-0**
RN 90764-56-0 CAOLD
CN L-Lysine, N6-(iodoacetyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```
=> d que stat l8
L8                STR

          9           10
          O           NH
          ‖           ⟆
          ‖           ⟅
I-~~CH2-C-~~NH~G1-~CH~C==O
1   2   3   4   5   6   7   8

REP G1=(3-4) CH2
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
```

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=> d his ful

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L8                STR
L9              3 SEA SSS SAM L8
L10            46 SEA SSS FUL L8

     FILE 'HCAPLUS' ENTERED AT 12:29:16 ON 22 APR 2004
L11            16 SEA ABB=ON  L10
L12            15 SEA ABB=ON  L11 NOT L7

     FILE 'CAOLD' ENTERED AT 12:30:28 ON 22 APR 2004
L13             1 SEA ABB=ON  L10
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15 hits in CA Plus with inventors not excluded

1 hit in CA Old ← See d que stat L8 for structure